Prediction of the energy efficiency of an Ar-H2-O2 plasma torch with Ansys Fluent

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Abstract

This study aims at modeling an inductively heated Ar-H2-O2 plasma [1]. This plasma produced by a plasma torch is commonly used for the removal of boron from Silicon [2]. Some modules made at SIMAP-EPM enable us to model the plasma specificities and the interaction of the conducting fluid with the electromagnetic field. The power generated by the coil will be partly dissipated with the joule effect in the conductive parts of the device, partly transmitted into the plasma. The energy transmitted into the plasma will be partly used for chemical reactions, partly used to heat the plasma. However the plasma will also transmit some of its energy to the water-cooled walls with the radiative effects. We define the energy efficiency R_{eff} as the fraction of plasma power provided by the torch to the reactor (in the form of an enthalpy flow and radiation flux). This study aims to predict this ratio for a given set of experiments [3].

Key words : Plasma torch – Energy efficiency – Argon – Hydrogen – Oxygen

Introduction

The improvement of the energy efficiency of silicon purification processes is critical to the competitiveness of photovoltaic energy. Silicon distillation processes, though able to produce high purity levels that fit the electronic industry, are too energy consuming. Lower requirements in purity for photovoltaic panels enable the exploration of other processes [4]. One of the latter steps of this chain of energy efficient processes is the removal of boron. The low segregation coefficient of boron makes solidification processes out of question. Therefore one of the main processes currently being explored at laboratory scale is the injection of an Ar-H2-O2 plasma over an inductively heated and stirred silicon melt. This plasma is produced with a torch that is using a coil at a frequency of 3.13 MHz and powers between 30 and 40 kW. In the industry, it is necessary to estimate which proportion of the energy used in the coil will actually be available at the torch outlet. Such estimates should be completed by estimates of how much energy will be used for the reactions inside the coil, particularly for the formation of O radicals and H radicals. A high enthalpy flow plasma also helps preventing the formation of silica particles at the surface of the melt.

Experimental Conditions

An induction coil surrounds the gas flow (fig.1). The induction coil is connected to a capacitance and a generator, which creates an oscillating current inside an LC circuit. This oscillating current creates an oscillating magnetic field parallel to the axis of the coil. This oscillating magnetic field accelerates the electrons, thus creating a current that counteracts the imposed magnetic field. The electrons collide with the gas molecules, which heats the gas molecules and ionizes a small fraction of the gas molecules. The gas has turned into a plasma [3]. At this moment, the plasma reaches inside the torch temperatures of over 10 000 K (fig.2). On the surface of the melt, the plasma will oxide the silicon and react with boron to form mainly HBO(g). The volume above the melt is named reactor. We are going to study the following experiments:

Experiment Name	Torch Power (kW)	Induction Frequency (MHz)	Ar flow (Nm3/h) F_{Ar}	H2 flow (Nm3/h) F_{H2}	O2 flow (Nm3/h) F_{O2}	R_{pow} =Power/ F_{total} in kWh/Nm3	R_{O+H} = $(F_{H2}+ F_{O2})/ F_{total}$
1 (MAIA)	38	3.13	7.33	0.31	0.06	4.9	0.05
2 (XXL 29)	33.4	3.13	4.90	0.126	0.025	6.6	0.03
3 (XXL 32)	34.1	3.13	4.37	0.249	0.023	7.3	0.06
4 (XXL 33)	33.8	3.13	4.69	0.246	0.026	6.8	0.06
5 (XXL 36)	33.8	3.13	4.72	0.126	0.025	6.9	0.03
6 (SUSImar02l)	38.4	3.13	6.3	0.4	0.1	5.6	0.08
7 (SuSImar02i)	42.4	3.13	6.3	1	0	5.8	0.16

Tab. 1 Experimental conditions

Numerical results

All the reactive, radiative, inductive, convective and transport phenomena including the Ar, H and O atoms have been modelized in details within specific modules added to Ansys Fluent ® [1].

For each experiment, with similar torch geometries, we are going to examine how the energy provided by the generator is spread into the torch (table1). First, there is the joule effect inside the coil and the power transmitted to the cold cage surrounding the plasma. This effect is taken into account by multiplicating the generator power with a coefficient, which is going to give us the plasma power used for the calculation (table 1). This coefficient has been adjusted to 0.5 from measurements of cooling heat fluxes [3]. Now let's examine how the plasma power is spread between the heat flux with the conduction and convection to the torch walls, the energy radiated to the torch walls, the energy radiated towards the reactor from the bottom of the torch and the energy provided in the form of enthalpy to the gases. Some of this enthalpy flow is being used to heat up the products (flow of sensible enthalpy, sensible enthalpy defined in equation 1), some of it is being used for chemical reactions to form new species (flow of enthalpy of reaction) (table 2). We are going to define the energy efficiency ratio R_{eff} as the fraction of plasma power provided by the torch to the reactor (in the form of an enthalpy flow and radiation flux).

Some definitions for Table2:

Sensible enthalpy:

$$h_S = \sum_{j \in species} \int_{T_{ref}}^{T} C_p^j dT \tag{1}$$

T_{ref} being the reference temperature

Enthalpy of reaction: change in the enthalpy of a chemical reaction that occurs at a constant pressure. It represents the amount of energy per mole either released or produced in a reaction.

In our case both enthalpies are calculated as a flow between the entrance of the torch and the bottom of the torch.

Net radiative energy provided to the reactor from the torch: energy radiated from the torch to the reactor minus energy radiated from the reactor to the torch. It may be negative because of the radiative energy from the melt.

kW / Exp number	1	2	3	4	5	6	7
Torch power	38.0	33.4	34.1	33.8	33.8	38.4	42.4
Plasma power	**19.0**	**16.7**	**17.0**	**16.9**	**16.9**	**19.2**	**21.2**
Energy radiated to the torch walls	4.35	4.4	4.2	4.3	4.2	3.0	3.8
Conducto-convection to the torch	3.6	2.2	3.0	2.6	2.6	2.6	6.2
Net radiative energy provided to the reactor from the torch	-0.14	0.1	0.001	0.04	0.1	1.2	-2.0
Flow of enthalpy	11.2	10.0	9.9	10.0	10.1	12.5	13.2
Energy Efficiency ratio R_{eff}	**0.58**	**0.61**	**0.58**	**0.60**	**0.60**	**0.71**	**0.53**

Tab 2: Energy fluxes from the torch

Analysis

The experiments 1 to 6 show an increase of the energy efficiency ratio R_{eff} (tab.2) when the ratio of reactive gases R_{O+H} (defined in tab. 1) increases (fig. 3). This increase can be linked to an increase in the rate of flow of enthalpy of reaction R_{reac} (defined in table 3) when R_{O+H} increases. This rate R_{reac} can be linked mainly to the very endothermic reactions of formation of radicals, found in high concentrations (fig. 6 and 7). Our interpretation is the following: an increase in R_{reac} means less energy is stored as sensible enthalpy, thus less energy is radiated by the plasma and less energy is lost through radiations towards the torch walls. We should also expect a decrease of R_{eff} when the torch power per flow unit R_{pow} (defined in table1) increases (fig. 5). This is because the hotter the plasma, the higher the losses through radiative emissions and conducto-convection through the torch walls. The correlation between lower temperatures, and lower radiative emissions can be seen in table 3 and correspond to higher R_{reac} coefficients.

We distinguish among the experiments and their simulations the experiment number 7 where Ar-H2 is injected from the experiments 1 to 6 where Ar-O2-H2 is injected. The positive correlation between R_{O+H} and R_{eff} cannot be found if we also consider the experiment 7, and the negative correlation between R_{eff} and R_{pow} is also less visible. One specificity of the experiment 7, is that contrary to all other experiments, its enthalpy losses are mostly due to conducto-convective losses inside the torch (tab. 2). We think that the high mass-diffusivity of some radicals H and protons H+, leads to a higher reactive thermal conductivity (eq. 2).

(2)

J_s represents the diffusion flux of species and h_s the molar enthalpy of species

This explains the high conducto-convective losses at the torch. At this point, we can wonder: why does this effect of high diffusivity of H species not work to this extent with the other experiments? There are two reasons, one reason is the lower concentration of hydrogen for the other experiments, the other reason is the presence of oxygen for experiments 1 to 6, for which the products have lower diffusivity. The influence due to the injection of O2 can be checked with the ratios R_{reac}/ R_{O+H} which represents the efficiency of reactive gazes to store enthalpy in the form of reaction enthalpy. This ratio is higher in the presence of oxygen and increases with the ratio of oxygen to hydrogen flow $R_{O/H}$ (table 3 and fig 4). We observe form tables 2 and 3 that $R_{O/H}$ is positively correlated with R_{eff} . The much bigger oxygen radicals or dioxygen molecules have lower diffusion coefficients than the much smaller hydrogen radicals and therefore contribute much less to the reactive thermal conductivity [5]. Therefore, in the presence of pure hydrogen, the enthalpy goes exclusively to the hydrogen products with higher diffusivity, which contribute more to the conductive heat transfers, hence the higher conductive losses and the lower R_{eff} ratio relative to the proportion of reactive gases injected, because less enthalpy is available for reactions. These higher losses reduce the efficiency R_{eff}.

KW / Exp number	1	2	3	4	5	6	7
Flow of enthalpy of reaction Q_R	1.8	1.3	1.7	1.8	1.5	2.6	3.7
Flow of sensible enthalpy Q_T	9.4	8.8	8.1	8.3	8.6	9.8	9.5
Total flow of enthalpy	**11.2**	**10**	**9.9**	**10.0**	**10.1**	**12.5**	**13.2**
$\mathbf{R_{reac}=Q_R/(Q_T+Q_R)}$	**0.16**	**0.13**	**0.18**	**0.18**	**0.14**	**0.21**	**0.28**
Average Temperature at Torch Outlet	4844	6620	6309	6245	6620	5380	4951
$\mathbf{R_{reac}/ R_{O+H}}$	3.4	4.25	3.01	3.21	4.65	2.85	2.03
$\mathbf{R_{O/H}=F_{O2}/F_{H2}}$	0.19	0.20	0.09	0.11	0.20	0.25	0

Tab. 3 Enthalpy of reaction and sensible enthalpy flows

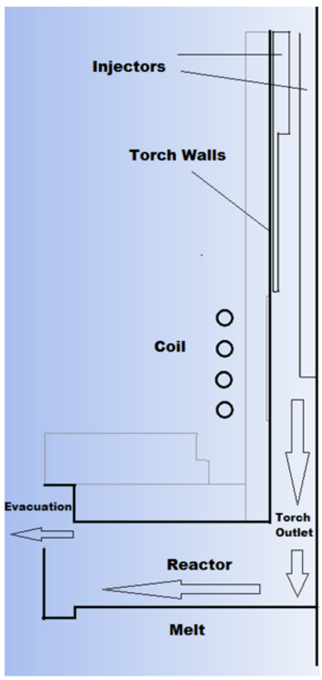

Fig. 1: Experimental Settings

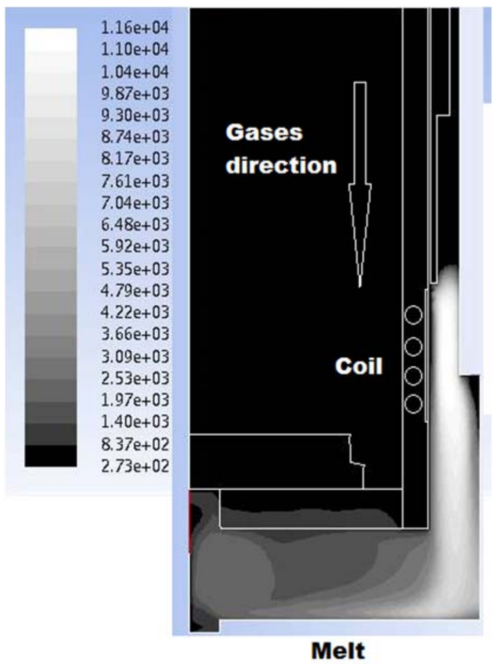

Fig. 2: Temperature Field

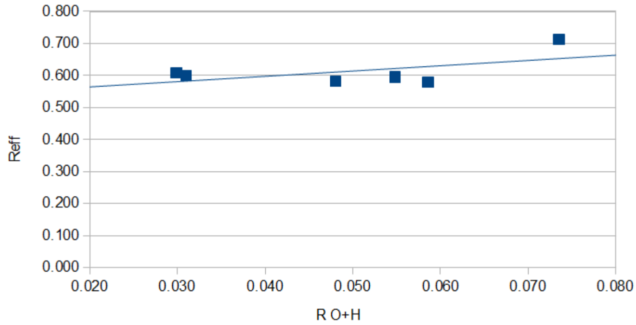

Fig. 3: Link between R_{O+H} and R_{eff} for experiments 1 to 6

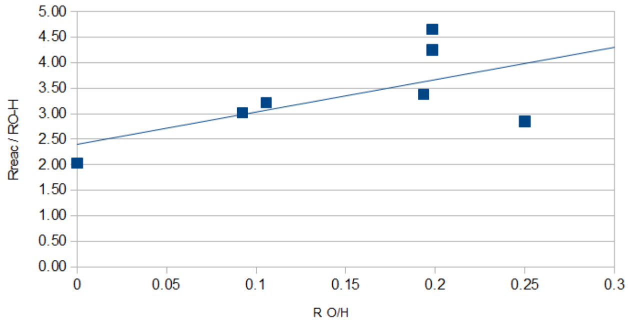

Fig. 4: Link between $R_{reac}/R_{O\text{-}H}$ and $R_{O/H}$

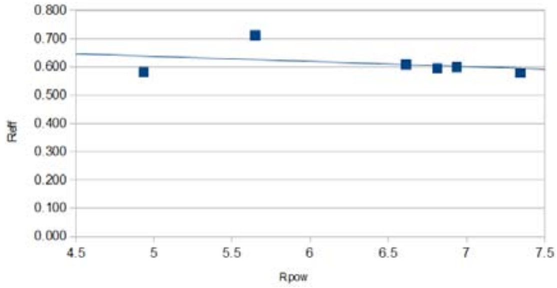

Fig. 5: Link between R_{pow} and R_{eff} (experiments 1 to 6)

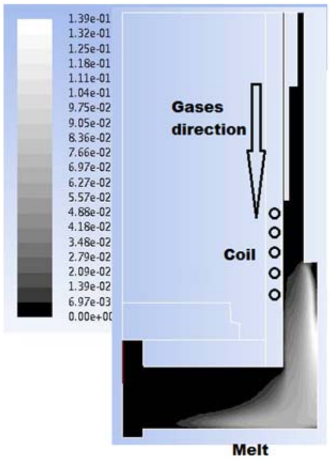

Fig 6: Mole Fraction of H radicals (experiment 5)

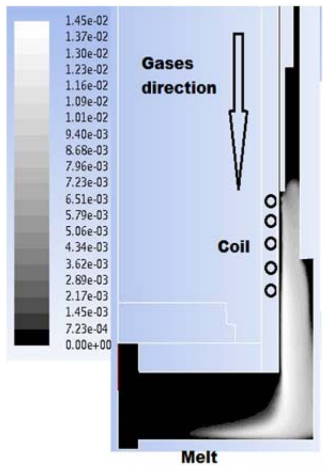

Fig. 7: Mole Fraction of O radicals (experiment 5)

Conclusion

We have made a numerical model of a set of seven experiments with inductively coupled plasma torches in the frame of the study of silicon purification. The mixture injected into the torch was either Ar-H2-O2 or Ar-H2. We found out that the formation of radicals was the main reason for important enthalpy storage. We also found out that this enthalpy storage was helping to make the process more efficient by decreasing the enthalpy losses to the torch walls through radiations or conducto-convective losses. However, this effect can be countered by conductive reactive heat losses due to the higher mass diffusivity for hydrogen radicals, ions or dihydrogen molecules than for oxygen radicals or ions, dioxygen or water molecules. Therefore, a higher content in oxygen seems to help to increase the efficiency ratio of Ar-H2-O2 plasma torches A more systematic numerical study with large variations of parameters may help to understand the phenomena better.

References

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